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Shooting and Embedding for Two-Point Boundary Value Problems*

HERBERT B. KELLER

Department of Applied Mathematics, California Institute of Technology, Pasadena, California 91109

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1. INTRODUCTION

The shooting method is an extremely powerful technique for both the theoretical analysis and approximate numerical solution of general two point boundary value problems. To illustrate we consider a problem of the form:

$$\text{(a)}\quad \mathbf{y}'(t) = \mathbf{F}(t, \mathbf{y}),\quad T_0 \leqslant t \leqslant T_1;\qquad \text{(b)}\quad \mathbf{B}(\mathbf{y}(T_0), \mathbf{y}(T_1)) = \mathbf{0}. \tag{1.1}$$

Here $\mathbf{y}$, $\mathbf{F}$ and $\mathbf{B}$ are, say, n-vector-valued functions of 1, $n+1$ and $2n$ arguments, respectively. We associate with (1.1) an initial value problem

$$\text{(a)}\quad \mathbf{Y}'(t) = \mathbf{F}(t, \mathbf{Y});\qquad \text{(b)}\quad \mathbf{Y}(T_0) = \mathbf{s}; \tag{1.2}$$

which under appropriate smoothness conditions on $\mathbf{F}$ has, for all $\mathbf{s}$ in some open set $S_0 \subset E^n$, a unique solution denoted by

$$\text{(c)}\qquad \mathbf{Y} \equiv \mathbf{Y}(t, \mathbf{s}). \tag{1.2}$$

If these solutions exist on $[T_0, T_1]$ then we may form

$$\text{(a)}\qquad \phi(\mathbf{s}) \equiv \mathbf{B}(\mathbf{s}, \mathbf{Y}(T_1, \mathbf{s})), \tag{1.3}$$

and note that a solution of (1.2) is also a solution of (1.1) for each $\mathbf{s} \in S_0$ which satisfies

$$\text{(b)}\qquad \phi(\mathbf{s}) = \mathbf{0}. \tag{1.3}$$

Conversely, if (1.1) has a solution $\mathbf{y}(t)$, then $\mathbf{s} = \mathbf{y}(T_0)$ is a root of (1.3b). Thus, by shooting, our two-point boundary value problem can be shown to

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be equivalent to the problem of solving the system (1.3b) of n equations in n unknowns on some set S_0. Obviously, various finite-dimensional fixed-point theorems can now be employed to study the existence theory for (1.1). If, in particular, some constructive fixed-point procedure is applicable, say, contraction mappings or Newton's method, then corresponding numerical methods are available which, in principle, yield accurate approximate solutions; see e.g. [3].

Of course, the shooting procedure (1.2), (1.3) could just as well be defined in reverse. That is, we associate with (1.1) the final value problem

$$\text{(a)} \quad \hat{\mathbf{Y}}'(t) = \mathbf{F}(t, \hat{\mathbf{Y}}), \qquad \text{(b)} \quad \hat{\mathbf{Y}}(T_1) = \mathbf{h}; \tag{1.4}$$

and denote the unique solution by

$$\text{(c)} \qquad \hat{\mathbf{Y}} \equiv \hat{\mathbf{Y}}(t, \mathbf{h}). \tag{1.4}$$

Then if the solution exists on $[T_0, T_1]$, for all $\mathbf{h}$ in some open set $H_0 \subset E^n$, we define

$$\text{(a)} \qquad \boldsymbol{\psi}(\mathbf{h}) \equiv \mathbf{B}(\hat{\mathbf{Y}}(T_0, \mathbf{h}), \mathbf{h}) \tag{1.5}$$

and the boundary value problem is reduced to solving

$$\text{(b)} \qquad \boldsymbol{\psi}(\mathbf{h}) = \mathbf{0}. \tag{1.5}$$

Existence theorems and numerical methods can be based equally well on solving (1.3b) or (1.5b). In practical computations, however, one or the other may be preferable—but these important considerations would take us too far astray.

Perhaps the most difficult step in the initial value program indicated above is the determination of some sufficiently small neighborhood S_0 in which a root of (1.3b) is to be found. For constructive methods (i.e., iterative schemes) this is equivalent to the choice of an initial iterate $\mathbf{s}^{(0)}$ leading to convergence. The more or less standard way to do this (especially in computations) is by some continuation or embedding process. That is, the original two-point problem depends upon or is made to depend upon some parameter or set of parameters in such a manner that it can easily be solved for a special value of the parameter set and so that the root $\mathbf{s}$ of (1.3b) depends upon the parameters in an appropriately smooth way. Then starting at the special parameter value, for which we can easily find $\mathbf{s}$, and using the smooth dependence of $\mathbf{s}$ on the parameters, we somehow continue (in small steps) to the desired parameter values. Obviously, the way in which the embedding parameters are introduced and used for continuation may be crucial in practice. These same considerations apply to the approach using final values, and, in fact, $\mathbf{h}$ will have the same smoothness properties with respect to the embedding parameters as those enjoyed by $\mathbf{s}$.

There are natural parameters that occur in all two-point boundary value problems—the points T_0 and T_1 at which the boundary constraints are applied, or, if $\mathbf{F}(t, \mathbf{y}) \equiv \mathbf{f}(\mathbf{y})$ is independent of t, the length of the interval, $T_1 - T_0$, between boundary points. When any of these parameters is employed for continuation and takes on a value which makes $T_1 - T_0 = 0$, then the boundary value problem degenerates to the simple problem of satisfying the boundary constraints with vectors $\mathbf{y}(T_0) \equiv \mathbf{y}(T_1)$. It is this fact and the continuous dependence upon the parameters that justifies the heuristic notion that boundary value problems are "easier" to solve over "shorter" intervals. Other parameters may occur and be equally significant in specific problems.

We use the right hand end point $T_1 = \tau$ as an embedding parameter and for generality we introduce p additional parameters $\boldsymbol{\xi}$ into both the differential equations and the boundary conditions. Then *we indicate how Newton's method and a continuation procedure in the $p + 1$ parameters $(\tau, \boldsymbol{\xi})$ can yield existence theorems and practical computing schemes.* The analysis of these procedures easily leads us to the derivation of a coupled system of first order quasilinear partial differential equations satisfied by the initial data $\mathbf{s}(\tau, \boldsymbol{\xi})$ and the final data $\mathbf{h}(\tau, \boldsymbol{\xi})$. Cauchy data are obtained for this system on $\tau = T_0$.

The coefficients in the above-indicated system of partial differential equations are not known explicitly in general. If the embedding parameters $\boldsymbol{\xi}$ only enter into the boundary conditions, and not into the differential equations, then all coefficients are given explicitly. *If the boundary conditions are of the separated endpoint form and satisfy some special solvability restrictions, then the system for* $\mathbf{s}$ *and* $\mathbf{h}$ *can be partially uncoupled and a system for* $\mathbf{h}$ *alone is obtained.* Here, as is rather obvious, $\mathbf{s}$ and $\mathbf{h}$ are of lower dimensionality and $\mathbf{h}$ enters only into the boundary conditions at $t = \tau$. The equation for $\mathbf{h}(\tau, \boldsymbol{\xi})$ is an obvious generalization of the so called embedding equation derived in studies of "invariant imbedding" [1, 6]. If the boundary conditions are of a special form or if $\boldsymbol{\xi}$ is introduced in a special way, our result reduces to the usual embedding equation. However, we find that *the characteristics of our more general embedding equations are not simply related to the integral curves of the system of embedded ordinary differential equations.*

We do not present detailed proofs in this paper but we do indicate the arguments that have been used to make it all quite rigorous. Fairly complete proofs of many of the results can be found in [3, 4] and especially [5]. Our rather discursive presentation is intended to get across the basic ideas without the lengthy interruptions that would be required to include proofs.

2. Embedding and Continuation

In place of the problem (1.1) we consider a family of boundary value problems

$$\text{(a)}\quad \mathbf{y}'(t) = \mathbf{F}(t, \mathbf{y}, \boldsymbol{\xi}), \quad T_0 \leqslant t \leqslant \tau; \qquad \text{(b)}\quad \mathbf{B}(\mathbf{y}(T_0), \mathbf{y}(\tau), \boldsymbol{\xi}) = 0. \tag{2.1}$$

Here $t = \tau$ is the right boundary point and $\boldsymbol{\xi}$ is a p-vector of parameters. If the parameters enter in such a way that for some special values, say, $\boldsymbol{\xi} = \mathbf{0}$ and $\tau = T_1$, the problem (2.1) becomes that in (1.1), then we say that the boundary value problem (1.1) is *embedded* in the $(p + 1)$-parameter family of problems (2.1). We consider the related family of initial value problems for $t \geqslant T_0$:

$$\text{(a)}\quad \mathbf{z}'(t) = \mathbf{F}(t, \mathbf{z}, \boldsymbol{\xi}), \qquad \text{(b)}\quad \mathbf{z}(T_0) = \mathbf{s}, \tag{2.2}$$

and denote the solution by

$$\text{(c)}\qquad \mathbf{z} \equiv \mathbf{z}(t, \boldsymbol{\xi}, \mathbf{s}). \tag{2 2}$$

Here n additional parameters $\mathbf{s}$ enter and *we assume that sufficient smoothness is imposed on* $\mathbf{F}(t, \mathbf{z}, \boldsymbol{\xi})$ *so that the solution* (2.2c) *exists on* $T_0 \leqslant t \leqslant \tau$ for all $\tau \in I_0 \subset E^1$, $\boldsymbol{\xi} \in D_0 \subset E^p$, $\mathbf{s} \in S_0 \subset E^n$. Furthermore, $\mathbf{z}(t, \boldsymbol{\xi}, \mathbf{s})$ is to be continuously differentiable with respect to $(t, \boldsymbol{\xi}, \mathbf{s}) \in I_0 \times D_0 \times S_0$. Then we can define

$$\text{(a)}\qquad \boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s}) \equiv \mathbf{B}(\mathbf{s}, \mathbf{z}(\tau, \boldsymbol{\xi}, \mathbf{s}), \boldsymbol{\xi}) \tag{2.3}$$

and a solution of (2.2) is also a solution of (2.1) provided

$$\text{(b)}\qquad \boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s}) = \mathbf{0}. \tag{2.3}$$

Newton's method is frequently a very powerful procedure for the theoretical and practical determination of a root $\mathbf{s} = \mathbf{s}(\tau, \boldsymbol{\xi})$ of (2.3b), and hence for solving the boundary value problem (2.1). We sketch its application here. With some initial estimate $\mathbf{s}^{(0)} = \mathbf{s}^{(0)}(\tau, \boldsymbol{\xi})$ of the root the Newton iterates $\{\mathbf{s}^{(\nu)}\}$ are defined by

$$\left.\begin{aligned} &\text{(a)} & \mathbf{s}^{(\nu+1)} &= \mathbf{s}^{(\nu)} + \Delta\mathbf{s}^{(\nu)} \\ &\text{(b)} & Q(\tau, \boldsymbol{\xi}, \mathbf{s}^{(\nu)})\, \Delta s^{(\nu)} &= -\, \boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s}^{(\nu)}) \end{aligned}\right\}\ \nu = 0, 1, 2, \ldots . \tag{2.4}$$

Here we have introduced the $n \times n$ Jacobian matrix

$$\begin{aligned} \text{(a)}\qquad Q(\cdot) &\equiv \frac{\partial \boldsymbol{\phi}(\cdot)}{\partial \mathbf{s}} \\ &= B_1(\mathbf{s}, \mathbf{z}(\cdot), \boldsymbol{\xi}) + B_2(\mathbf{s}, \mathbf{z}(\cdot), \boldsymbol{\xi})\, Z(\cdot), \end{aligned} \tag{2.5}$$

where

$$\text{(b)}\quad (\cdot) \equiv (\tau, \xi, \mathbf{s}), \qquad B_1 \equiv \frac{\partial \mathbf{B}}{\partial \mathbf{s}} \ \text{ is } \ n \times n, \qquad B_2 \equiv \frac{\partial \mathbf{B}}{\partial \mathbf{z}} \ \text{ is } \ n \times n$$

$$Z(\cdot) \equiv \frac{\partial \mathbf{z}(\cdot)}{\partial \mathbf{s}} \ \text{ is } \ n \times n.$$

By formal differentiation in (2.2) we obtain the linear variational system for the $n \times n$ Jacobian $Z(t) \equiv Z(t, \xi, \mathbf{s})$:

$$Z'(t) = \frac{\partial \mathbf{F}(t, \mathbf{z}(t, \xi, \mathbf{s}), \xi)}{\partial \mathbf{z}} Z(t), \qquad Z(T_0) = I. \tag{2.6}$$

To justify the above definitions, we need only to require that $\mathbf{F}(t, \mathbf{z}, \xi)$ and $\mathbf{B}(\mathbf{s}, \mathbf{z}, \xi)$ have continuous derivatives with respect to their arguments on appropriate domains. Then to determine one iterate $\mathbf{s}^{(\nu)}$ we must first solve the single nonlinear initial value problem (2.2) and the n linear initial value problems (2.6). Conditions insuring the nonsingularity of $Q(\cdot)$ are somewhat complicated and closely related to the convergence proof for Newton's method [3-5]. Of course, it is clear from continuity that if $Q(\tau, \xi, \mathbf{s})$ is nonsingular for $\mathbf{s} = \mathbf{s}^{(0)}$, then the same holds for all $\mathbf{s}$ in some small sphere about $\mathbf{s}^{(0)}$. *The convergence proofs essentially use this fact and thus require the determination of an appropriate initial point* $\mathbf{s}^{(0)}(\tau, \xi)$. *Then using additional hypothesis* (see [4]), *it is shown that the iterates* $\mathbf{s}^{(\nu)}$ *do not deviate too far from* $\mathbf{s}^{(0)}$ *so that the* $Q(\tau, \xi, \mathbf{s}^{(\nu)})$ *are also nonsingular. Finally, the iterates, which are now well defined, are shown to form a Cauchy sequence whose limit is a unique root of* (2.3b) (*in the small sphere about* $s^{(0)}$).

Let us assume that for the parameter value $(\tau, \xi) = (\tau_0, \xi_0) \in I_0 \times D_0$ a root of (2.3b), $\mathbf{s} = \mathbf{s}_0 \in S_0$, is determined. If at this root $Q(\tau_0, \xi_0, \mathbf{s}_0)$ is nonsingular (as will be the case if Newton's method converges), then the Implicit Function theorem is applicable. This assures us that (2.3b) *has a unique root, say,*

$$\mathbf{s} = \mathbf{s}(\tau, \xi) \in S_0 \tag{2.7a}$$

depending continuously on (τ, ξ) *in some neighborhood* $N(\tau_0, \xi_0) \subset I_0 \times D_0$. *This root satisfies* $\mathbf{s}(\tau_0, \xi_0) = \mathbf{s}_0$, *and*

$$\phi(\tau, \xi, \mathbf{s}(\tau, \xi)) = \mathbf{0} \qquad \textit{for all } (\tau, \xi) \in N(\tau_0, \xi_0). \tag{2.7b}$$

The root $\mathbf{s}(\tau, \xi)$ is even Lipschitz continuously differentiable if the same is true of $\mathbf{F}$ and $\mathbf{B}$. The neighborhood $N(\tau_0, \xi_0)$ is not restricted to be small but extends in all directions until either the continuity, differentiability, or nonsingularity condition is violated. In the latter case, roots may continue to exist but cease to be unique, and solutions to the boundary value problem may then branch or bifurcate. (These interesting topics will be treated elsewhere.)

Contracting maps can be employed to prove the Implicit Function theorem [2], and so they can also be used to determine $\mathbf{s}(\tau, \boldsymbol{\xi})$ on $N(\tau_0, \boldsymbol{\xi}_0)$. Of course, the contractions are only valid in a small neighborhood of some existing root and the global results are obtained by a process of continuation. In practical computations, Newton's method may be preferable since the convergence is usually quadratic.

A basic point both in the convergence proof hinted at above for Newton's method and in the global Implicit Function theorem application is the determination of an *appropriate* initial iterate $\mathbf{s}^{(0)} = \mathbf{s}^{(0)}(\tau, \boldsymbol{\xi})$ for whatever iteration scheme is employed at the parameter value $(\tau, \boldsymbol{\xi})$. In actual computations, this choice is frequently crucial. In terms of the root $\mathbf{s}_0 = \mathbf{s}(\tau_0, \boldsymbol{\xi}_0)$ at $(\tau_0, \boldsymbol{\xi}_0)$, an obvious choice is $\mathbf{s}^{(0)}(\tau, \boldsymbol{\xi}) \equiv \mathbf{s}_0$ provided $(\tau, \boldsymbol{\xi})$ is sufficiently close to $(\tau_0, \boldsymbol{\xi}_0)$. This *continuation procedure* is sometimes called *the continuity method*, since its validity depends only upon the continuity of $\mathbf{s}(\tau, \boldsymbol{\xi})$ near $(\tau_0, \boldsymbol{\xi}_0)$. However, we can obtain much better estimates by simply using two terms of the Taylor expansion as in

$$\begin{aligned} \mathbf{s}^{(0)}(\tau, \boldsymbol{\xi}) &\equiv \mathbf{s}_0 + \frac{\partial \mathbf{s}(\tau_0, \boldsymbol{\xi}_0)}{\partial \tau}(\tau - \tau_0) + \frac{\partial \mathbf{s}(\tau_0, \boldsymbol{\xi}_0)}{\partial \boldsymbol{\xi}}(\boldsymbol{\xi} - \boldsymbol{\xi}_0) \\ &= \mathbf{s}(\tau, \boldsymbol{\xi}) + \mathcal{O}(|\tau - \tau_0|^2 + |\boldsymbol{\xi} - \boldsymbol{\xi}_0|^2). \end{aligned} \tag{2.8}$$

This expansion and remainder estimate follow from the Implicit Function theorem, as in (2.7), provided that $\mathbf{F}$ and $\mathbf{B}$ are, say, twice continuously differentiable.

To apply (2.8) we must determine the derivatives $\partial \mathbf{s}/\partial \tau$ and $\partial \mathbf{s}/\partial \boldsymbol{\xi}$. Since (2.7b) is an identity on $N(\tau_0, \boldsymbol{\xi}_0)$, differentiation with respect to τ and $\boldsymbol{\xi}$ yields

$$\frac{\partial \boldsymbol{\phi}(*)}{\partial \tau} + \frac{\partial \boldsymbol{\phi}(*)}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \tau} = 0, \qquad \frac{\partial \boldsymbol{\phi}(*)}{\partial \boldsymbol{\xi}} + \frac{\partial \boldsymbol{\phi}(*)}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \boldsymbol{\xi}} = 0, \tag{2.9a}$$

where the argument is

$$(*) \equiv (\tau, \boldsymbol{\xi}, \mathbf{s}(\tau, \boldsymbol{\xi})). \tag{2.9b}$$

Thus it follows that if $Q(*) \equiv \partial \boldsymbol{\phi}(*)/\partial \mathbf{s}$ is nonsingular, we can solve (2.9) for the coefficients in (2.8). Of course, the *nonsingularity of Q was also required in Newton's method as well as in the Implicit Function theorem*; so we do not impose any new conditions. Recalling (2.3a), (2.5), and (2.6), we obtain, on solving (2.9a),

$$\begin{aligned} \frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \tau} &= -Q^{-1}(*)\, B_2(**)\, \mathbf{F}(\tau, \mathbf{z}(*), \boldsymbol{\xi}), \\ \frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}} &= -Q^{-1}(*)\, [B_2(**)\, W(*) + B_3(**)], \end{aligned} \tag{2.10a}$$

where

$$(**) \equiv (\mathbf{s}(\tau, \boldsymbol{\xi}), \mathbf{z}(*), \boldsymbol{\xi}),$$
$$B_3 \equiv \frac{\partial \mathbf{B}}{\partial \boldsymbol{\xi}} \quad \text{is} \quad n \times p, \qquad W \equiv \frac{\partial \mathbf{z}}{\partial \boldsymbol{\xi}} \quad \text{is} \quad n \times p. \tag{2.10b}$$

By formal differentiation in (2.2), we get the variational system for $W(t) \equiv W(t, \boldsymbol{\xi}, \mathbf{s})$:

$$W'(t) = \frac{\partial \mathbf{F}(t, \mathbf{z}(t, \boldsymbol{\xi}, \mathbf{s}), \boldsymbol{\xi})}{\partial \mathbf{z}} W(t) + \frac{\partial \mathbf{F}(t, \mathbf{z}(t, \boldsymbol{\xi}, \mathbf{s}), \boldsymbol{\xi})}{\partial \boldsymbol{\xi}}; \qquad W(T_0) = 0. \tag{2.11}$$

It is important to note here that if $\mathbf{F}$ is independent of $\boldsymbol{\xi}$, then $W \equiv 0$ and the expression for $\partial \mathbf{s}/\partial \boldsymbol{\xi}$ simplifies considerably. In this case *the derivates* (2.10a) *are determined by the data required in Newton's method.* Then (2.8) is the natural continuation procedure to use in specifying initial data for Newton's method.

Suppose the parameters $\boldsymbol{\xi} \in E^p$ have $p = n$; that is, dim $\boldsymbol{\xi} =$ dim $\mathbf{s}$. Then the matrix

$$P(*) \equiv \frac{\partial \boldsymbol{\phi}(*)}{\partial \boldsymbol{\xi}} = [B_2(**)\, W(*) + B_3(**)] \tag{2.12}$$

is $n \times n$. If det $P(*) \neq 0$, we may eliminate $Q(*)$ in (2.10a) to get

$$\frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \tau} = \frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}} P^{-1}(*)\, B_2(**)\, \mathbf{F}(\tau, \mathbf{z}(*), \boldsymbol{\xi}). \tag{2.13}$$

This is a quasilinear first-order system of partial differential equations satisfied by $\mathbf{s}(\tau, \boldsymbol{\xi})$. However, the coefficients are not explicitly known functions of $(\tau, \boldsymbol{\xi}, \mathbf{s})$ by virtue of their dependence on $W(*)$ and $\mathbf{z}(*)$. We shall remedy this situation in part by considering the final value procedure.

3. Final Values and Generalized Embedding Equations

The continuation procedures of Section 2 yield solutions of the boundary value problem (2.1) for all $(\tau, \boldsymbol{\xi}) \in N(\tau_0, \boldsymbol{\xi}_0)$ by means of $\mathbf{s}(\tau, \boldsymbol{\xi})$ and the initial value problem (2.2). However, as observed in Section 1, we could just as well employ final value problems (i.e., shooting in the opposite direction), say, for $t \leqslant \tau$,

$$\text{(a)} \quad \hat{\mathbf{z}}' = \mathbf{F}(t, \hat{\mathbf{z}}, \boldsymbol{\xi}); \qquad \text{(b)} \quad \hat{\mathbf{z}}(\tau) = \mathbf{h}. \tag{3.1}$$

For existence theorems and practical computations we could apply our previous analysis to determine appropriate final values $\mathbf{h} = \mathbf{h}(\tau, \boldsymbol{\xi})$ so that the solution of (3.1), say,

$$\text{(c)} \qquad \hat{\mathbf{z}}(t) = \hat{\mathbf{z}}(t, \boldsymbol{\xi}, \mathbf{h}, \tau), \tag{3.1}$$

satisfies

$$\boldsymbol{\psi}(\tau, \boldsymbol{\xi}, \mathbf{h}) \equiv \mathbf{B}(\hat{\mathbf{z}}(T_0, \boldsymbol{\xi}, \mathbf{h}, \tau), \mathbf{h}, \boldsymbol{\xi}) = \mathbf{0}. \tag{3.2}$$

Essentially, nothing new is obtained in this exercise although it is very important to point out that in practice the two procedures may by no means be equally effective (see the discussion in [3]). Note that the τ dependence of $\hat{\mathbf{z}}$ is much different from that of $\mathbf{z}$.

From the analysis in Section 2 we easily see that the correct final data, for which the solution of (3.1) will satisfy (3.2), must be

$$\mathbf{h}(\tau, \boldsymbol{\xi}) = \mathbf{z}(\tau, \boldsymbol{\xi}, \mathbf{s}(\tau, \boldsymbol{\xi})) \equiv \mathbf{z}(*) \qquad \text{for all } (\tau, \boldsymbol{\xi}) \in N(\tau_0, \boldsymbol{\xi}_0). \tag{3.3}$$

[Conversely, if $\mathbf{h}(\tau, \boldsymbol{\xi})$ is known, then $\mathbf{s}(\tau, \boldsymbol{\xi}) = \hat{\mathbf{z}}(T_0, \boldsymbol{\xi}, \mathbf{h}(\tau, \boldsymbol{\xi}), \tau)$ and we have the interesting identities on $N(\tau_0, \boldsymbol{\xi}_0)$:

$$\mathbf{h}(\tau, \boldsymbol{\xi}) = \mathbf{z}(\tau, \boldsymbol{\xi}, \hat{\mathbf{z}}[T_0, \boldsymbol{\xi}, h(\tau, \boldsymbol{\xi}), \tau)]), \qquad \mathbf{s}(\tau, \boldsymbol{\xi}) = \hat{\mathbf{z}}(T_0, \boldsymbol{\xi}, \mathbf{z}[\tau, \boldsymbol{\xi}, \mathbf{s}(\tau, \boldsymbol{\xi})], \tau).$$

We shall not pursue the consequences of these identities in this paper.] By differentiation in (3.3) we get, recalling (2.2), (2.5b), and (2.10b),

$$\begin{aligned} \frac{\partial \mathbf{h}(\tau, \boldsymbol{\xi})}{\partial \tau} &= \mathbf{F}(\tau, \mathbf{h}(\tau, \boldsymbol{\xi}), \boldsymbol{\xi}) + Z(*) \frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \tau}, \\ \frac{\partial \mathbf{h}(\tau, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}} &= W(*) + Z(*) \frac{\partial \mathbf{s}(\tau, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}}. \end{aligned} \tag{3.4}$$

Again, let us require that $p = n$ and that the resulting $n \times n$ matrix $P(*)$ in (2.12) is nonsingular. Then (2.13) is valid and with this in (3.4) we get, on eliminating $Z(*)\, \partial \mathbf{s}/\partial \boldsymbol{\xi}$,

$$\frac{\partial \mathbf{h}}{\partial \tau} = \left[\frac{\partial \mathbf{h}}{\partial \boldsymbol{\xi}} - W(*)\right] P^{-1}(*)\, B_2(**)\, \mathbf{F}(\tau, \mathbf{h}, \boldsymbol{\xi}) + \mathbf{F}(\tau, \mathbf{h}, \boldsymbol{\xi}). \tag{3.5}$$

We recall that $(*) = (\tau, \boldsymbol{\xi}, \mathbf{s}(\tau, \boldsymbol{\xi}))$ and $(**) = (\mathbf{s}(\tau, \boldsymbol{\xi}), \mathbf{h}(\tau, \boldsymbol{\xi}), \boldsymbol{\xi})$ since $\mathbf{z}(*) = \mathbf{h}(\tau, \boldsymbol{\xi})$. Thus $\mathbf{s}(\tau, \boldsymbol{\xi})$ and $\mathbf{h}(\tau, \boldsymbol{\xi})$ satisfy the coupled quasilinear first-order system of partial differential equations (2.13) and (3.5). Since the matrix function $W(\tau, \boldsymbol{\xi}, \mathbf{s})$ is not known in general, this system has, at best, formal siginficance.

However we recall that *if the parameters* ξ *do not enter into the differential equations* (2.1) but only into the boundary conditions, then $\partial \mathbf{F}/\partial \xi \equiv 0$ and so by (2.11), $W \equiv 0$. *In this case* (2.13) *and* (3.5) *reduce to the explicit quasilinear system*

$$\begin{aligned} &\text{(a)} && \frac{\partial \mathbf{s}}{\partial \tau} = \frac{\partial \mathbf{s}}{\partial \xi} B_3^{-1}(\mathbf{s}, \mathbf{h}, \xi)\, B_2(\mathbf{s}, \mathbf{h}, \xi)\, \mathbf{F}(\tau, \mathbf{h}), \\ &\text{(b)} && \frac{\partial \mathbf{h}}{\partial \tau} = \frac{\partial \mathbf{h}}{\partial \xi} B_3^{-1}(\mathbf{s}, \mathbf{h}, \xi)\, B_2(\mathbf{s}, \mathbf{h}, \xi)\, \mathbf{F}(\tau, \mathbf{h}) + \mathbf{F}(\tau, \mathbf{h}). \end{aligned} \tag{3.6}$$

By considering the limiting case $\tau \to T_0$, we may obtain a Cauchy problem for this system provided $(T_0, \xi) \in N(\tau_0, \xi_0)$ for some ξ domain. In this limit the boundary value problem (2.1) degenerates, since there is no interval over which to satisfy the differential equation, and we need only satisfy the boundary conditions

$$\mathbf{B}(\mathbf{s}, \mathbf{h}, \xi) = 0.$$

However, we must also have, from the definitions of $\mathbf{s}$ and $\mathbf{h}$,

$$\mathbf{s}(T_0, \xi) = \mathbf{h}(T_0, \xi).$$

Thus *if there is a root* $\eta = \eta(\xi)$ *of*

$$\text{(a)} \qquad \mathbf{B}(\eta, \eta, \xi) = 0, \tag{3.7}$$

then the Cauchy data for (3.6) *are, on* $\tau = T_0$,

$$\text{(b)} \qquad \mathbf{s}(T_0, \xi) = \eta(\xi), \qquad \mathbf{h}(T_0, \xi) = \eta(\xi). \tag{3.7}$$

It is by no means clear that any practical advantage has been gained in replacing the two-point boundary value problem (2.1) by the Cauchy problem (3.6)–(3.7). But the latter is a pure initial value problem for a system of partial differential equations. So *we have shown in a very general setting that this can be done.* If the Cauchy problem can be solved in some (τ, ξ) domain, say by the Cauchy–Kowalewski expansion (assuming analyticity), or by the method of characteristics, then (2.1) can be solved for all (τ, ξ) in this domain. It is not difficult to show that this is the case, but, of course, we must assume the nonsingularity of various matrices, as was done in the derivation of (3.6). We shall not take the time here for this argument; see [6] for the general idea.

The embedding parameters ξ *may be introduced in a manner which simplifies* (3.6) *further*. For example, if in terms of the boundary conditions of (1.1), we define

$$\mathbf{B}(\mathbf{s}, \mathbf{h}, \xi) \equiv \mathbf{B}(\mathbf{s}, \mathbf{h}) + \xi,$$

then $B_3(\mathbf{s}, \mathbf{h}, \boldsymbol{\xi}) = I$, the $n \times n$ identity matrix. Of course, in this case the point $(\tau, \boldsymbol{\xi}) = (T_1, \mathbf{0})$ must be included in the solution domain of our Cauchy problem in order to solve the original two-point boundary value problem. Another important special case is that of linear boundary conditions, say,

$$\mathbf{B}(\mathbf{s}, \mathbf{h}, \boldsymbol{\xi}) \equiv B_1\mathbf{s} + B_2\mathbf{h} + B_3\boldsymbol{\xi},$$

where B_3 is nonsingular. Then $B_3^{-1}B_2$ in (3.6) is just a constant $n \times n$ matrix. We shall see in the next section that for some boundary conditions of the separated endpoint type it is possible to uncouple the equation for $\mathbf{h}$ from any dependence upon $\mathbf{s}$ and to introduce $\boldsymbol{\xi}$ so that $B_3^{-1}(\mathbf{s}, \mathbf{h}, \boldsymbol{\xi})\, B_2(\mathbf{s}, \mathbf{h}, \boldsymbol{\xi}) = I$. *It is this special case that is called "invariant imbedding" in the literature* [1, 6].

4. Special Separated Endpoint Conditions and Invariant Imbedding

Separated endpoint conditions are quite common. That is m conditions are imposed on $\mathbf{y}(T_0)$ and $p = n - m$ conditions are imposed on $\mathbf{y}(T_1)$. With little or no loss in generality we can assume that the conditions at $t = T_0$ can be solved for m fixed components of $\mathbf{y}$, say, the first m components, in terms of the remaining p components. Then if we use the decomposition $\mathbf{y} \equiv \binom{\mathbf{u}}{\mathbf{v}}$ where $\mathbf{u} \in E^m$ and $\mathbf{v} \in E^p$ the boundary condition at $t = T_0$ has the form

$$\mathbf{u}(T_0) = \mathbf{a}(\mathbf{v}(T_0)),$$

where $\mathbf{a}$ is an m-vector-valued function. *We also require, with much greater loss in generality, that the condition at $t = T_1$ can be solved for the last p components in terms of the first m components.* Thus in the above notation these conditions have the form

$$\mathbf{v}(T_1) = \mathbf{b}(\mathbf{u}(T_1)).$$

This latter restriction on the boundary conditions is not very natural although it occurs frequently in specific applications. We impose it here as it is sufficient for uncoupling the generalized embedding Eqs. (3.6). Perhaps this could be proven necessary too, but at present this is an open question.

The differential equations in (1.1) can be written in the decomposed form

$$\text{(a)} \qquad \mathbf{u}'(t) = \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \qquad \mathbf{v}'(t) = \mathbf{g}(t, \mathbf{u}, \mathbf{v}), \tag{4.1}$$

where $\mathbf{F} \equiv \binom{\mathbf{f}}{\mathbf{g}}$, $\mathbf{f} \in E^m$ and $\mathbf{g} \in E^p$. We embed this system subject to the above boundary conditions in a $p + 1$ parameter family of boundary value problems by imposing the boundary conditions

$$\text{(b)} \qquad \mathbf{u}(T_0) = \mathbf{a}(\mathbf{v}(T_0)), \qquad \mathbf{v}(\tau) = \mathbf{b}(\mathbf{u}(\tau), \boldsymbol{\xi}). \tag{4.1}$$

Here $\boldsymbol{\xi} \in E^p$, and we assume that for some special value of $\boldsymbol{\xi}$, say, $\boldsymbol{\xi} = \mathbf{0}$, $\mathbf{b}(\mathbf{u}, \mathbf{0}) \equiv \mathbf{b}(\mathbf{u})$.

Now we proceed exactly as in Sections 2 and 3, shooting from $t = T_0$ with initial values $\mathbf{V}(T_0) = \mathbf{s} \in E^p$ and $\mathbf{U}(T_0) = \mathbf{a}(\mathbf{s}) \in E^m$ and seek $\mathbf{s}$ to satisfy

$$\boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s}) \equiv \mathbf{V}(\tau, \mathbf{s}) - \mathbf{b}(\mathbf{U}(\tau, \mathbf{s}), \boldsymbol{\xi}) = \mathbf{0}, \tag{4.2}$$

where $(\mathbf{U}(t, \mathbf{s}), \mathbf{V}(t, \mathbf{s}))$ is the solution of the indicated initial value problem. The Implicit Function theorem will be valid if there is a root $(\tau_0, \boldsymbol{\xi}_0)$ and the $p \times p$ Jacobian matrix

$$Q(\tau, \boldsymbol{\xi}, \mathbf{s}) \equiv \frac{\partial \boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s})}{\partial \mathbf{s}} = \frac{\partial \mathbf{V}(\tau, \mathbf{s})}{\partial \mathbf{s}} - \frac{\partial \mathbf{b}(\mathbf{U}(\tau, \mathbf{s}), \boldsymbol{\xi})}{\partial \mathbf{U}} \frac{\partial \mathbf{U}(\tau, \mathbf{s})}{\partial \mathbf{s}}$$

is nonsingular in some domain $N(\tau_0, \boldsymbol{\xi}_0)$. If in this neighborhood $\mathbf{s} = \mathbf{s}(\tau, \boldsymbol{\xi})$ is the root of (4.2), then from the identity $\boldsymbol{\phi}(\tau, \boldsymbol{\xi}, \mathbf{s}(\tau, \boldsymbol{\xi})) = 0$ we obtain

$$\frac{\partial \mathbf{s}}{\partial \tau} = -Q^{-1}(*) \frac{\partial \boldsymbol{\phi}(*)}{\partial \tau}, \qquad \frac{\partial \mathbf{s}}{\partial \boldsymbol{\xi}} = -Q^{-1}(*) \frac{\partial \boldsymbol{\phi}(*)}{\partial \boldsymbol{\xi}},$$

and thus

$$\frac{\partial \mathbf{s}}{\partial \tau} = \frac{\partial \mathbf{s}}{\partial \boldsymbol{\xi}} \left(\frac{\partial \boldsymbol{\phi}(*)}{\partial \boldsymbol{\xi}} \right)^{-1} \frac{\partial \boldsymbol{\phi}(*)}{\partial \tau}. \tag{4.3}$$

Here we have, from (4.2),

$$\frac{\partial \boldsymbol{\phi}(*)}{\partial \boldsymbol{\xi}} = -\frac{\partial \mathbf{b}(\mathbf{U}(\tau, \mathbf{s}), \boldsymbol{\xi})}{\partial \boldsymbol{\xi}},$$

$$\frac{\partial \boldsymbol{\phi}(*)}{\partial \tau} = g(\tau, \mathbf{U}(\tau, \mathbf{s}), \mathbf{V}(\tau, \mathbf{s})) - \frac{\partial \mathbf{b}(\mathbf{U}(\tau, \mathbf{s}), \boldsymbol{\xi})}{\partial \mathbf{U}} \mathbf{f}(\tau, \mathbf{U}(\tau, \mathbf{s}), \mathbf{V}(\tau, \mathbf{s})),$$

and it is assumed that $\partial \boldsymbol{\phi}(*)/\partial \boldsymbol{\xi}$ is nonsingular. [Eq. (4.3) is the counterpart of (2.13).]

From the analogous final value problem associated with (4.1) and taking final values $\hat{\mathbf{U}}(\tau) = \mathbf{h} \in E^m$ and $\hat{\mathbf{V}}(\tau) = \mathbf{b}(\mathbf{h}, \boldsymbol{\xi}) \in E^p$, we find that

$$\boldsymbol{\psi}(\tau, \boldsymbol{\xi}, \mathbf{h}) \equiv \hat{\mathbf{U}}(T_0, \boldsymbol{\xi}, \mathbf{h}, \tau) - \mathbf{a}(\hat{\mathbf{V}}(T_0, \boldsymbol{\xi}, \mathbf{h}, \tau)) = 0,$$

provided

$$\mathbf{h}(\tau, \boldsymbol{\xi}) = \mathbf{U}(\tau, \mathbf{s}(\tau, \boldsymbol{\xi})). \tag{4.4a}$$

Since this is an identity on $N(\tau_0, \boldsymbol{\xi}_0)$, we now get

$$\frac{\partial \mathbf{h}}{\partial \tau} = \frac{\partial \mathbf{U}(\tau, \mathbf{s})}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \tau} + f(\tau, \mathbf{U}(\tau, \mathbf{s}), \mathbf{V}(\tau, \mathbf{s})), \qquad \frac{\partial \mathbf{h}}{\partial \boldsymbol{\xi}} = \frac{\partial \mathbf{U}(\tau, s)}{\partial \mathbf{s}} \frac{\partial \mathbf{s}}{\partial \boldsymbol{\xi}}.$$

Thus with the aid of (4.3) this yields

$$\frac{\partial \mathbf{h}}{\partial \tau} = \frac{\partial \mathbf{h}}{\partial \boldsymbol{\xi}} \left(\frac{\partial \phi(*)}{\partial \boldsymbol{\xi}}\right)^{-1} \frac{\partial \phi(*)}{\partial \tau} + \mathbf{f}(\tau, \mathbf{U}(\tau, \mathbf{s}), \mathbf{V}(\tau, \mathbf{s})).$$

It follows from (4.2) and (4.4a) that

$$\mathbf{V}(\tau, \mathbf{s}(\tau, \boldsymbol{\xi})) = \mathbf{b}(\mathbf{h}(\tau, \boldsymbol{\xi}), \boldsymbol{\xi}). \tag{4.4b}$$

Note that (4.4a, b) determine $\mathbf{U}(\tau, \mathbf{s}(\tau, \xi))$ and $\mathbf{V}(\tau, \mathbf{s}(\tau, \xi))$ in terms of $\boldsymbol{\xi}$ and $\mathbf{h}(\tau, \boldsymbol{\xi})$. Using these relations, we find that the equation for h is uncoupled from any dependence on $\mathbf{s}$; specifically, with (4.4) we get

$$\begin{aligned}\frac{\partial \mathbf{h}}{\partial \tau} = &- \frac{\partial \mathbf{h}}{\partial \boldsymbol{\xi}} \left[\frac{\partial \mathbf{b}(\mathbf{h}, \boldsymbol{\xi})}{\partial \boldsymbol{\xi}}\right]^{-1} \left[\mathbf{g}(\tau, \mathbf{h}, \mathbf{b}(\mathbf{h}, \boldsymbol{\xi})) - \frac{\partial \mathbf{b}(\mathbf{h}, \boldsymbol{\xi})}{\partial \mathbf{h}} \mathbf{f}(\tau, \mathbf{h}, \mathbf{b}(\mathbf{h}, \boldsymbol{\xi}))\right] \\ &+ \mathbf{f}(\tau, \mathbf{h}, \mathbf{b}(\mathbf{h}, \boldsymbol{\xi})).\end{aligned} \tag{4.5}$$

A very interesting special case of the embedding in (4.1b) is the choice $\mathbf{b}(\mathbf{u}(\tau), \boldsymbol{\xi}) \equiv \mathbf{b}(\mathbf{u}(\tau)) + \boldsymbol{\xi}$ as then $\partial \mathbf{b}/\partial \boldsymbol{\xi} = I$, the $p \times p$ identity. Still more special is the case in which $\mathbf{v}(T_1) = \boldsymbol{\alpha}$, say, is specified as the boundary condition at $t = T_1$. Then if we take $\mathbf{b}(\mathbf{u}, \boldsymbol{\xi}) \equiv \boldsymbol{\xi}$, we also get $\partial \mathbf{b}/\partial \mathbf{u} = 0$ and (4.5) becomes in this case

$$\frac{\partial \mathbf{h}}{\partial \tau} + \frac{\partial \mathbf{h}}{\partial \xi} \mathbf{g}(\tau, \mathbf{h}, \boldsymbol{\xi}) = \mathbf{f}(\tau, \mathbf{h}, \boldsymbol{\xi}). \tag{4.6}$$

This is the more or less familiar equation of invariant imbedding. Of course it can also be relevant for general boundary conditions of the form $\mathbf{v}(T_1) = \mathbf{b}(\mathbf{u}(T_1))$ by simply employing the embedding $\mathbf{v}(\tau) = \boldsymbol{\xi}$ in $(4.1\dot{\text{b}})$. But then solutions of (4.6) do not directly yield solutions of the boundary value problem of interest. This occurs only for those $\boldsymbol{\xi}$ which satisfy $\boldsymbol{\xi} = \mathbf{b}(\mathbf{h}(\tau, \boldsymbol{\xi}))$; see [6] for a detailed study of this approach. It is only in these somewhat special cases that the characteristics of the embedding equation are also integral curves of the original ordinary differential equation. In particular, the characteristics of (4.5) depend in general upon $\mathbf{b}(\mathbf{u}, \boldsymbol{\xi})$, which occurs in the boundary conditions (4.1b). Thus the characteristics are not simply integral curves of (4.1a).

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